Succinic acid, 2,3-dichlorobenzyl 2-methylhex-3-yl ester

Inchi: InChI=1S/C18H24Cl2O4/c1-4-6-15(12(2)3)24-17(22)10-9-16(21)23-11-13-7-5-8-14(19)18

InchiKey: XTRJYPSDAYZTPJ-UHFFFAOYSA-N

Formula: C18H24Cl2O4

SMILES: CCCC(OC(=O)CCC(=O)OCc1cccc(Cl)c1Cl)C(C)C

Mol. weight [g/mol]: 375.29

Physical Properties

Property code	Value	Unit	Source
gf	-302.75	kJ/mol	Joback Method
hf	-732.90	kJ/mol	Joback Method
hfus	42.56	kJ/mol	Joback Method
hvap	85.57	kJ/mol	Joback Method
log10ws	-5.92		Crippen Method
logp	5.185		Crippen Method
mcvol	280.080	ml/mol	McGowan Method
pc	1466.85	kPa	Joback Method
rinpol	2479.00		NIST Webbook
rinpol	2479.00		NIST Webbook
tb	874.44	K	Joback Method
tc	1088.12	K	Joback Method
tf	518.24	K	Joback Method
vc	1.069	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	813.55	J/mol×K	874.44	Joback Method
cpg	869.65	J/mol×K	1052.50	Joback Method
cpg	860.66	J/mol×K	1016.89	Joback Method
cpg	850.57	J/mol×K	981.28	Joback Method
cpg	839.37	J/mol×K	945.67	Joback Method
cpg	827.04	J/mol×K	910.05	Joback Method
cpg	877.56	J/mol×K	1088.12	Joback Method
dvisc	0.0000460	Pa×s	874.44	Joback Method

dvisc	0.0000595	Pa×s	815.07	Joback Method
dvisc	0.0000801	Pa×s	755.71	Joback Method
dvisc	0.0001135	Pa×s	696.34	Joback Method
dvisc	0.0001717	Pa×s	636.97	Joback Method
dvisc	0.0002828	Pa×s	577.61	Joback Method
dvisc	0.0005220	Pa×s	518.24	Joback Method

Sources

Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U380887&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume